

Triprolidine  
486-12-4 | DTXSID3023718

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 346 °C

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 5.59e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4,4'-Methylenebis(N,N-dimethylaniline)</div> <div>Measured: 390</div> <div>Predicted: 349</div>	<div>Image not found</div> <div>Imazalil</div> <div>Measured: 347</div> <div>Predicted: 338</div>	<div>Image not found</div> <div>1,3-Dimethyl-1,3-diphenylurea</div> <div>Measured: 350</div> <div>Predicted: 338</div>
<div>Image not found</div> <div>3,5-Diphenyl-1,2,4-oxadiazole</div> <div>Measured: 290</div> <div>Predicted: 317</div>	<div>Image not found</div> <div>2,2'-Dinitrobiphenyl</div> <div>Measured: 305</div> <div>Predicted: 327</div>	